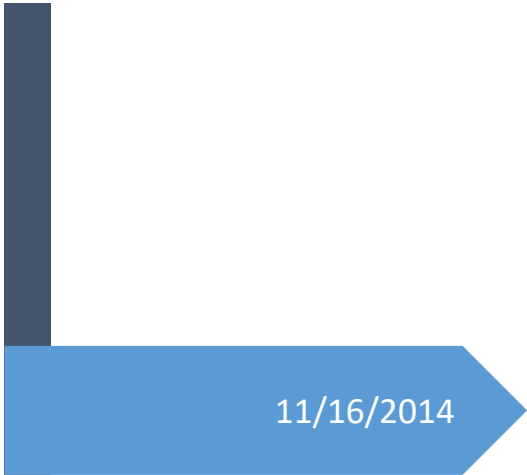
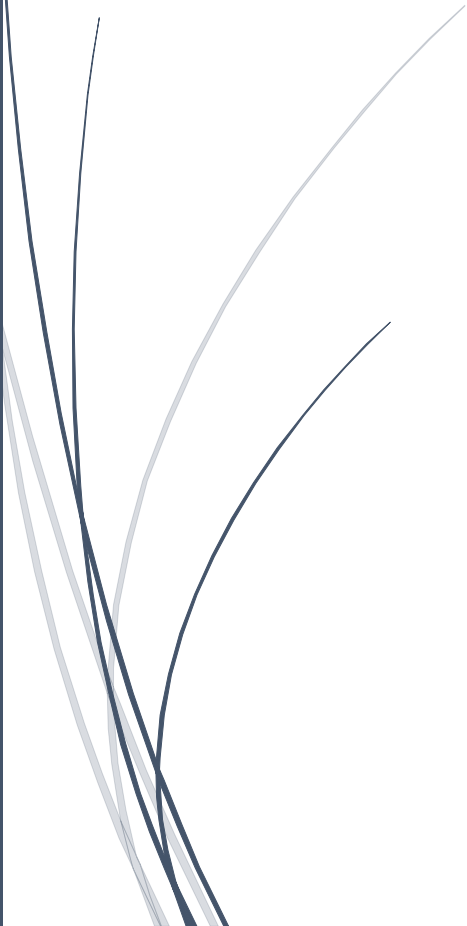


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11/16/2014

DP Notes Part 2

Extra Notes by Pratik Gautam

Several thin, curved lines in dark blue and light grey originate from the bottom left corner and sweep upwards and to the right.

This notebook belongs to Siddhant Rimal

$$= \int_{-\infty}^{\infty} (\pi \psi_1(x))^* \psi_2(x) dx$$

Q.E.D.

③ Parity operator commutate with Hamiltonian.

$$[\hat{\pi}, \hat{H}_x] = 0$$

$$\hat{H}_x = \frac{p_x^2}{2m} + V(x)$$

$$= \frac{\left(-i\hbar \frac{d}{dx}\right)^2}{2m} + V(x)$$

$$\hat{H}_x = \frac{-\hbar^2 d^2}{2m dx^2} + V(x)$$

Proof:

$$\hat{H}_x \psi(x) = -\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} + V(x) \psi(x)$$

multiplying with $\hat{A}$,

$$\hat{A} H_x \psi(x) = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(-x) + V(-x) \psi(-x)$$

$$= \left\{ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(-x) \right\} \psi(-x)$$

$$= \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right) \pi \psi(x)$$

$$\therefore V(x) = V(-x)$$

$$\hat{A} H_x \psi(x) = H_x \hat{A} \psi(x)$$

$$(\hat{A} H_x - H_x \hat{A}) \psi(x) = 0$$

$$[\hat{A}, H_x] \psi(x) = 0$$

$$\Rightarrow [\hat{A}, H_x] = 0 \quad \psi(x) \neq 0$$

proved.

7 postulates.

Postulates of Quantum Mechanics

Postulate I: It describes about the wave function. It describes the wave function as a mathematical expn which deals with the space time behaviour of the particle.

Postulate II

It deals with the Superposition principle. It means that if ψ_1 and ψ_2 are the two state function for different state of a system. Then $\psi = A_1\psi_1 + A_2\psi_2$ where A_1 and A_2 are the constants.

Postulate III

It states that each dynamical variable in quantum mechanics has its own respective operator which is operated to the wave function results the measurable quantity.

Postulate IV

It states about each eigen value operator when operated to the eigen value wave function it results eigen value times the same wave function i.e. $\boxed{\hat{A}\psi = \lambda\psi}$.

Postulate V:

It deals with the average of all the measurement for a physical quantity is called the expectation of that quantity and it is defined as

$$\langle A \rangle = \int_{-\infty}^{\infty} \psi^* \hat{A} \psi dx$$

↓
Expectation
value of
dynamical
~~value~~
variable.

Postulate VI:- It deals with the prob. of finding the particle in the given space. When the wave function is multiplied with its conjugate it gives a quantity called prob density.

ie

$$\psi^* \psi = \text{prob. density}$$

When it is integrated over the specified ~~to~~ region it results

$$\int_{-\infty}^{\infty} \psi^* \psi \cdot dv = 1$$

Postulate VII:

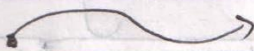
It describes the characteristics of the wavefunctions ie the wave function is continuous & single valued which also means that its first order derivative is also continuous.

Free particle, potential = 0.

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Application of Schrodinger Wave eqn

(i) Free Particle!


m, v
free particle

Let m be the mass of free particle, moving along x-axis with velocity v. Then the Schrodinger wave eqn

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} = E \psi \quad \text{where } \psi \text{ is wave fn.}$$

$$\text{or, } \frac{d^2 \psi}{dx^2} = -\frac{2mE}{\hbar^2} \psi$$

$$\text{or } \frac{d^2 \psi}{dx^2} + \frac{2mE}{\hbar^2} \psi = 0$$

$$\text{or } \frac{d^2 \psi}{dx^2} + k^2 \psi = 0 \quad \text{--- (1)}$$

$$\text{where, } k^2 = \frac{2mE}{\hbar^2} \quad \text{--- (2)}$$

$$\begin{array}{l} \text{~~~~~} \rightarrow Ae^{ikx} \\ \text{~~~~~} \rightarrow Be^{-ikx} \end{array}$$

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The soln of eqn (i) be written as,

$$\psi = Ae^{ikx} + Be^{-ikx}$$

The entire soln including time be written as,

$$\boxed{\psi(x,t) = (Ae^{ikx} + Be^{-ikx}) e^{-i\omega t}}$$

If wave is travelling along the x-axis then,

$$\psi(x,t) = Ae^{ikx} e^{-i\omega t}$$

$$\psi(x,t) = A e^{-i(\omega t - kx)}$$

The prob. density defined as,

$$P = \int_{-\infty}^{\infty} A^* e^{i(\omega t - kx)} A e^{-i(\omega t - kx)} dx$$

$$P = |A|^2 \int_{-\infty}^{\infty} dx$$

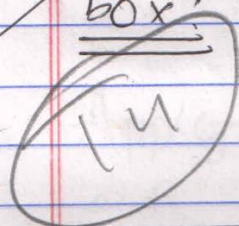
$$\therefore P = \infty$$

Which is not possible because we have assumed the ideal case

ie, $V=0$ [potential is zero].
~~which concludes potential less~~
~~particle is not possible in the~~
~~universe.~~

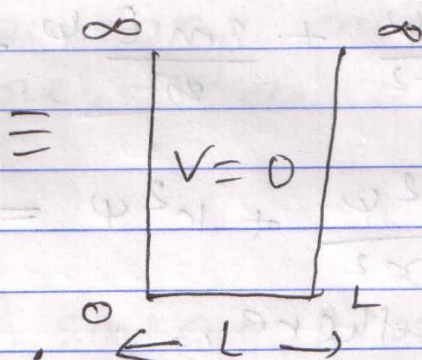
② Particle Bounded in one dimensional box:

Imp



A B

metallic
wire



1D potential well

Fig: 1D box.

$$V(x) = 0 ; 0 \leq x \leq L$$

$$= \infty ; \text{elsewhere}$$

Motion of an electron in a metallic wire is assumed as particle bounded in 1D box. The system is defined as,

$$V(x) = 0 \quad ; \quad 0 \leq x \leq L$$

$$= \infty \quad ; \quad \text{elsewhere}$$

where L is the length of the wire.
The Schrodinger wave eqⁿ,

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} = E \psi \quad (\text{Time indep. SWT})$$

$$\text{or } \frac{d^2 \psi}{dx^2} + \frac{2mE}{\hbar^2} \psi = 0$$

$$\Rightarrow \frac{d^2 \psi}{dx^2} + k^2 \psi = 0 \quad \text{--- (1)}$$

where,

$$k^2 = \frac{2mE}{\hbar^2} \quad \text{--- (2)}$$

The solⁿ of this eqⁿ (1) be written as,

$$\boxed{\psi(x) = A \sin kx + B \cos kx} \quad \text{--- (3)}$$

where A and B are ~~some~~ constant.

Particle exists within the box only
ie

$$\psi(x) \Big|_{x=0} = 0$$

and

$$\psi(x) \Big|_{x=L} = 0$$

Applying boundary conditions,
of above, at $x=0$,

we get,

$$\psi(0) = A \sin k(0) + B \cos k(0)$$

$$0 = 0 + B$$

$$\therefore \boxed{B = 0}$$

Using the value of B in eqn (3),
we get,

$$\psi(x) = A \sin kx$$

Again apply 2nd condⁿ at $x=L$,

Particle exists within the box only
ie

$$\psi(x) \Big|_{x=0} = 0$$

and

$$\psi(x) \Big|_{x=L} = 0$$

Applying boundary conditions,
of above, at $x=0$,

we get,

$$\psi(0) = A \sin k(0) + B \cos k(0)$$

$$0 = 0 + B$$

$$\therefore \boxed{B = 0}$$

Using the value of B in eqn (3),
we get,

$$\psi(x) = A \sin kx$$

Again apply 2nd condn at $x=L$,

$$\psi(L) = A \sinh kL + B \cos$$

$$\psi(L) = A \sin kL$$

$$0 = A \sin kL$$

$$A \neq 0$$

$$\Rightarrow \sin kL = 0$$

$$\Rightarrow \sin kL = \sin n\pi; \quad n = 0, 1, 2, \dots$$

$$\Rightarrow kL = n\pi$$

$$\therefore k = \frac{n\pi}{L}$$

Then,

eqn 4 becomes,

$$\boxed{\psi(x) = A \sin \frac{n\pi x}{L}}$$

Normalizing, we get,

$$\int_0^L \psi^* A \psi(x) dx = 1$$

$$\odot \int_0^L \frac{A \sin \frac{n\pi x}{L}}{L} \frac{A \sin \frac{n\pi x}{L}}{L} dx = 1$$

$$\odot |A|^2 \int_0^L \frac{\sin^2 \frac{n\pi x}{L}}{L} dx = 1$$

$$\odot |A|^2 \int_0^L \frac{(1 - \cos^2 \frac{n\pi x}{L})}{2} dx = 1$$

$$\odot \frac{|A|^2}{2} \int_0^L dx = 1$$

$$\odot \frac{|A|^2 (L)}{2} = 1$$

$$|A| = \sqrt{\frac{2}{L}}$$

Thus,

$$\psi(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \quad \text{--- (5)}$$

$$n = 1, 2, 3, \dots$$

1 = ground state
2 = 1st ~~ground~~ state.
excited

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In general,

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi}{L} x$$

$$\Rightarrow \psi_1(x) = \sqrt{\frac{2}{L}} \sin \frac{\pi}{L} x$$

$$\Rightarrow \psi_2(x) = \sqrt{\frac{2}{L}} \sin \frac{2\pi}{L} x$$

Using the value of k in eqn (2)
we get,

$$k^2 = \frac{2mE}{\hbar^2}$$

$$\left(\frac{n\pi}{L}\right)^2 = \frac{2mE}{\hbar^2}$$

$$E = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$

for $n = 1, 2, 3, 4, \dots$

$$\text{for } n=1, E_1 = \frac{\pi^2 \hbar^2}{2mL^2} \quad [\text{ground state}]$$

for $n=2$,

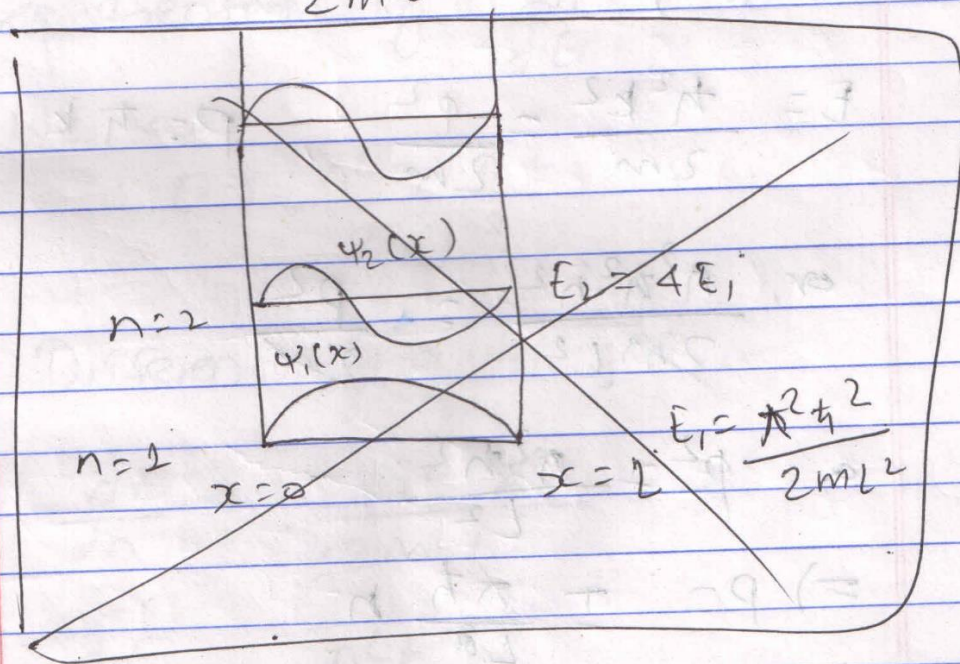
$$E_2 = \frac{4\pi^2\hbar^2}{2mL^2} = 4E_1 \quad (\text{first excited state})$$

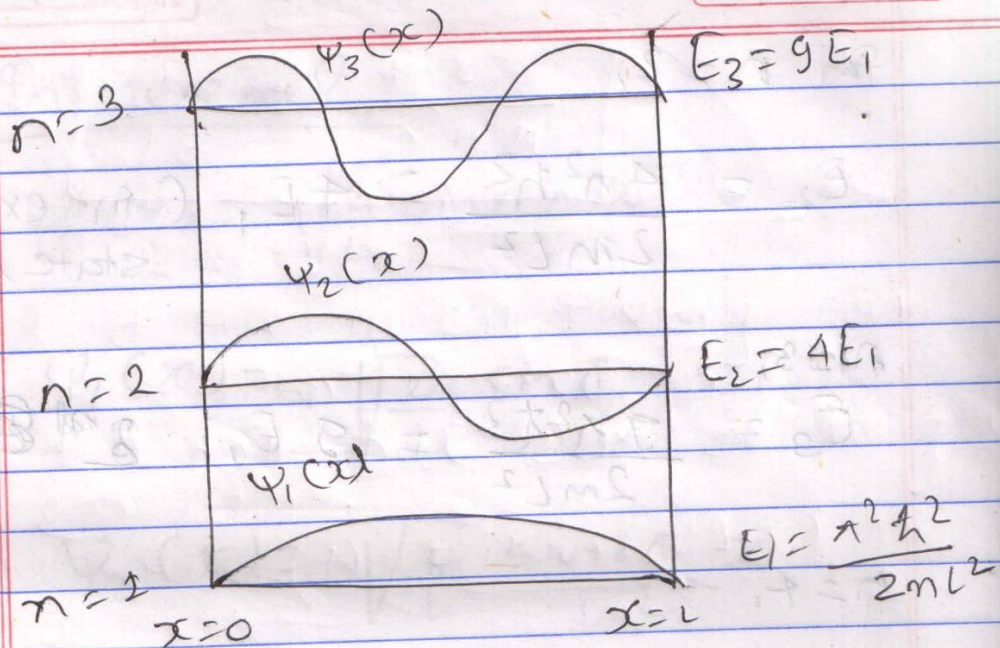
$n=3$,

$$E_3 = \frac{9\pi^2\hbar^2}{2mL^2} = 9E_1, \quad 2^{\text{nd}} \text{ E.S.}$$

$n=4$,

$$E_4 = \frac{16\pi^2\hbar^2}{2mL^2} = 16E_1 = 3^{\text{rd}} \text{ E.S.}$$





further,

$$E = \frac{\hbar^2 k^2}{2m} = \frac{p^2}{2m} ; \quad p = \hbar k$$

$$\text{or, } \frac{\pi^2 \hbar^2 n^2}{2mL^2} = \frac{p^2}{2m}$$

$$\Rightarrow p^2 = \frac{\pi^2 \hbar^2 n^2}{L^2}$$

$$\Rightarrow p = \pm \frac{\pi \hbar n}{L}$$

$$E_n = n^2 E_1$$

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Positive value of momentum means motion of particle along positive x-axis. and negative value of momentum means motion of particle along -ve x-axis.

Density of state: / Energy state

It is defined as the total n. of energy state per unit energy interval. It is represented by $\frac{dn}{dE}$

We have,

$$E = \frac{n^2 h^2 \pi^2}{2mL^2}$$

Differentiating we get,

$$\frac{dE}{dn} = \frac{\pi^2 h^2 \pi^2}{2mL^2} \cdot 2n$$

$$\frac{dE}{dn} = \frac{\pi^2 h^2 \pi^2 n}{mL^2}$$

$$\left(\hbar = \frac{h}{2\pi} \right)$$

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$$\therefore \frac{dn}{dE} = \frac{m L^2}{\pi^2 \hbar^2 n}$$

- (Q1) Find the lowest energy of an electron confined to move in 1D potential box of length ~~10~~ $1 \text{ \AA}$.

Given $(1 \text{ eV} = 1.6 \times 10^{-19} \text{ J})$

Soln

Here

$$n = 1$$

$$\hbar = 6.62 \times 10^{-34} \text{ JS}$$

$$m = 9.1 \times 10^{-31} \text{ kg}$$

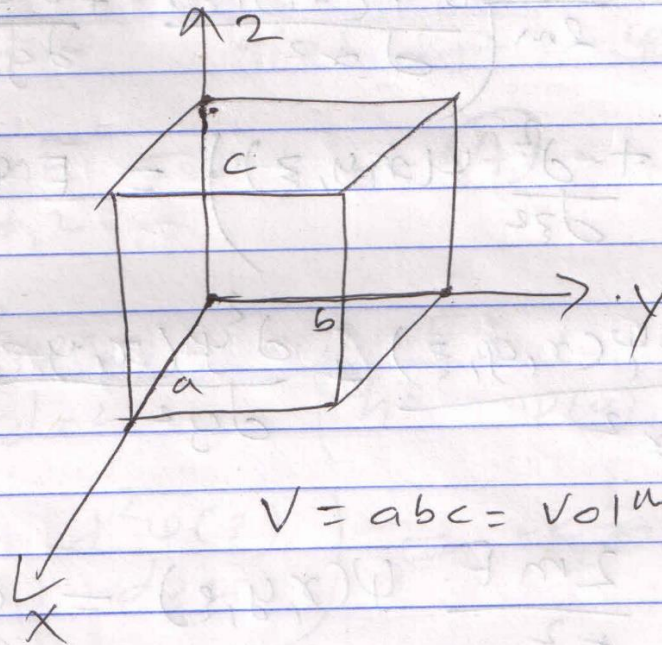
Now we have,

$$E_1 = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$

$$E_1 = \frac{(3.14)^2 \times \left(\frac{6.62 \times 10^{-34}}{2 \times 3.14} \right)^2}{2 \times 9.1 \times 10^{-31} \times (1 \times 10^{-10})^2}$$

$$\therefore E_1 = 6 \times 10^{-18} \text{ J}$$

Motion of particle confined in 3D box



Consider a 3D box as shown in fig. Let a particle having mass m be confined in it. This system be defined as

$$V(x, y, z) = \begin{cases} 0 & , 0 \leq x \leq a \\ & , 0 \leq y \leq b \\ & ; 0 \leq z \leq c. \\ \infty & \text{elsewhere.} \end{cases}$$

SWE for this system be written as

$$-\frac{\hbar^2}{2m} \left(\frac{\partial^2 \psi(x, y, z)}{\partial x^2} + \frac{\partial^2 \psi(x, y, z)}{\partial y^2} + \frac{\partial^2 \psi(x, y, z)}{\partial z^2} \right) = E \psi(x, y, z)$$

$$9 \quad \frac{\partial^2 \psi(x, y, z)}{\partial x^2} + \frac{\partial^2 \psi(x, y, z)}{\partial y^2} + \frac{\partial^2 \psi(x, y, z)}{\partial z^2} + \frac{2mE}{\hbar^2} \psi(x, y, z) = 0$$

$$+ \frac{2mE}{\hbar^2} \psi(x, y, z) = 0$$

$$\text{Let } \psi(x, y, z) = \psi(x) \psi(y) \psi(z)$$

$$\psi_y \psi_z \frac{\partial^2 \psi(x)}{\partial x^2} + \psi(x) \psi_z \frac{\partial^2 \psi(y)}{\partial y^2}$$

$$+ \psi(x) \psi(y) \frac{\partial^2 \psi(z)}{\partial z^2} + \frac{2mE}{\hbar^2} \psi(x) \psi(y) \psi(z) = 0$$

$$\psi(y) \psi(z) = 0$$

Dividing by $\psi(x) \psi(y) \psi(z)$, we get,

$$\frac{1}{\psi(x)} \frac{d^2 \psi(x)}{dx^2} + \frac{1}{\psi(y)} \frac{d^2 \psi(y)}{dy^2} + \frac{1}{\psi(z)} \frac{d^2 \psi(z)}{dz^2} + \frac{2mE}{\hbar^2} = 0 \quad \text{--- (A)}$$

$$\Rightarrow \frac{1}{\psi(x)} \frac{d^2 \psi(x)}{dx^2} = - \left(\frac{2mE}{\hbar^2} + \frac{1}{\psi(y)} \frac{d^2 \psi(y)}{dy^2} + \frac{1}{\psi(z)} \frac{d^2 \psi(z)}{dz^2} \right) = -k_x^2 \text{ (say)}$$

$$\Rightarrow \frac{1}{\psi(x)} \frac{d^2 \psi(x)}{dx^2} = -k_x^2 \quad \text{--- (1)}$$

Similarly

$$\frac{1}{\psi(y)} \frac{d^2 \psi(y)}{dy^2} = -k_y^2 \quad \text{--- (2)}$$

$$\frac{1}{\psi(z)} \frac{d^2 \psi(z)}{dz^2} = -k_z^2 \quad \text{--- (3)}$$

And, eqn (A) becomes,

$$-k_x^2 - k_y^2 - k_z^2 + \frac{2mE}{\hbar^2} = 0$$

$$\Rightarrow k_x^2 + k_y^2 + k_z^2 = \frac{2mE}{\hbar^2}$$

$$\text{or } E = \frac{\hbar^2}{2m} (k_x^2 + k_y^2 + k_z^2) \quad \text{--- (4)}$$

$$k_x = \frac{n_x \pi}{a},$$

$$k_y = \frac{n_y \pi}{b}$$

$$k_z = \frac{n_z \pi}{c}$$

$$\therefore E = \frac{\hbar^2}{2m} \left(\frac{n_x^2 \pi^2}{a^2} + \frac{n_y^2 \pi^2}{b^2} + \frac{n_z^2 \pi^2}{c^2} \right)$$

$$E = \frac{\hbar^2 \pi^2}{2m} \left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2} \right)$$

In general,

$$E_{n_x n_y n_z} = \frac{\hbar^2 \pi^2}{2m} \left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2} \right)$$

for cubical box $a=b=c$

$$E_{n_x n_y n_z} = \frac{\hbar^2 \pi^2}{2ma^2} (n_x^2 + n_y^2 + n_z^2)$$

The expression for the wave function, be written as

$$\psi_{n_x}(x) = A \sin k_x x$$

$$\psi_{n_y}(y) = B \sin k_y y$$

$$\psi_{n_z}(z) = C \sin k_z z$$

on combining we get,

$$\psi_{n_x n_y n_z}(x, y, z) = (ABC) \sin k_x x \sin k_y y \sin k_z z$$

after normalizing we get,

$$\psi_{n_x n_y n_z}(x, y, z) = \sqrt{\frac{2}{a}} \sqrt{\frac{2}{b}} \sqrt{\frac{2}{c}} \sin k_x x \sin k_y y \sin k_z z$$

$$\therefore \psi_{n_x n_y n_z}(x, y, z) = \sqrt{\frac{8}{abc}} \frac{\sin n_x x}{a} \frac{\sin n_y y}{b} \frac{\sin n_z z}{c}$$

for cubical box,

$$a = b = c$$

$$\psi_{n_x n_y n_z}(x, y, z) = \sqrt{\frac{8}{a^3}} \frac{\sin n_x x}{a} \frac{\sin n_y y}{a} \frac{\sin n_z z}{a}$$

is eigen wave fn.

Degeneracy

$$E_{n_x n_y n_z} = \frac{h^2 \pi^2}{2ma^2} [n_x^2 + n_y^2 + n_z^2]$$

for $n_x = 1$

$n_y = 1$

$n_z = 1$

first eigen value

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✓ $E_{111} = \frac{\hbar^2 \pi^2}{2ma^2} \cdot 3$ ground state energy.

for $n_x=1, n_y=2, n_z=1$

$E_{121} = \frac{\hbar^2 \pi^2}{2ma^2} [6]$, its excited state.

for $n_x=2, n_y=1, n_z=1$

$E_{211} = \frac{\hbar^2 \pi^2}{2ma^2} [6]$, its excited state.

and $n_x=1, n_y=1, n_z=2$

$E_{112} = \frac{\hbar^2 \pi^2}{2ma^2} [6]$

for the different values of states if there exists the same energy, then value then it is called degenerate state and such condition is called degeneracy.

Eg: E_{121}, E_{112} and E_{211} are degenerate energy states.

Q. Find the lowest energy of an electron confined in a cubical box of side $1\text{\AA}$.

Soln

Given,
 $a = 1 \times 10^{-10} \text{ m}$

We know

$$E = \frac{h^2 \pi^2}{2ma^2} (n_x^2 + n_y^2 + n_z^2)$$

for lowest $n_x = 1 = n_y = n_z$

$$E = \frac{6.62 \times 10^{-34} (3.14)^2 (1^2 + 1^2 + 1^2)}{2 \times 9.1 \times 10^{-31} \times (1 \times 10^{-10})^2}$$

$$\therefore E =$$

Q. find the lowest energy of an electron confined to move in 1D Box. of length $1 \text{ \AA}$.

$$E = \frac{h^2 \pi^2 n^2}{2ma^2} \quad n=1$$

$$E = \frac{(6.62 \times 10^{-34})^2 (3.14)^2}{2 \times 9.1 \times 10^{-31} \times (1 \times 10^{-10})^2}$$

$$\therefore E =$$

Q. find the temp at which the average ~~of~~ energy of molecule of a perfect gas would be equal to lowest energy of electron. the size of box in which confined is $1 \text{ \AA}$.

Soln

The lowest energy state in the cubical box.

$$E_{III} = \frac{\hbar^2 \pi^2}{2m a^2} (1^2 + 1^2 + 1^2)$$

Now,

$$E_{III} = \frac{3}{2} k_B T = 3$$

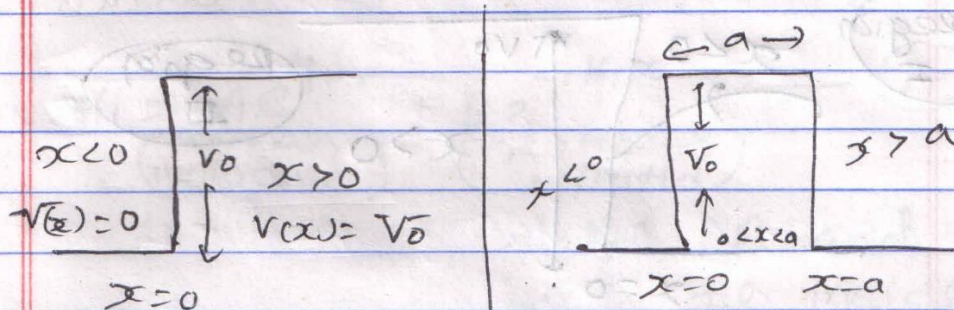
$$Q \quad \frac{\hbar^2 \pi^2}{2m a^2} \cancel{3} = \frac{\cancel{3} k_B T}{\cancel{2}} = 3$$

$$Q5 \quad T = \frac{\hbar^2 \pi^2}{m a^2 k_B}$$

$$Q \quad T = \frac{(6.62 \times 10^{-34})^2 (3.14)^2}{(9.1 \times 10^{-31}) (1 \times 10^{-10})^2 1.38 \times 10^{-23}}$$

$$T = 8.71 \times 10^5 \text{ K}$$

Potential Barrier and potential step



fig(i) potential step

potential barrier

Potential step: It is a system for the existence of potential in which the value of potential increases abruptly and goes forever.

Potential barrier: It is system for the existence of potential in which the potential exists upto a fixed value.

Potential step:

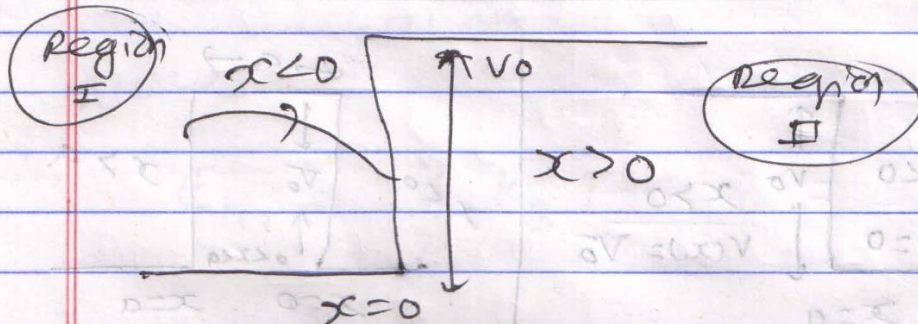


fig (i) potential step.

let the beam of particles of mass m incident on the potential step as shown in fig with $E > V_0$

The SWE for region I,

$$\frac{d^2 \psi_I}{dx^2} + \frac{2m}{\hbar^2} (E - V_0) \psi_I = 0$$

$$\text{or } \frac{d^2 \psi_I}{dx^2} + \frac{2m}{\hbar^2} E \psi_I = 0$$

$$\text{or } \frac{d^2 \psi_I}{dx^2} + k_1^2 \psi_I = 0 \quad \text{--- (1)}$$

$$; k_1^2 = \frac{2mE}{\hbar^2} \quad \text{--- (2)}$$

The soln of equation (i) be written as,

$$\psi_I = A e^{ik_1 x} + B e^{-ik_1 x} \quad \text{--- (A)}$$

(represents incident) (represents reflected)

where, A and B are the incident and reflected ~~mod~~ amplitude.

The SWE for region II,

$$\frac{d^2 \psi_{II}}{dx^2} + \frac{2m}{\hbar^2} (E - V_0) \psi_{II} = 0$$

$$\text{or, } \frac{d^2 \psi_{II}}{dx^2} + k_2^2 \psi_{II} = 0 \quad \text{--- (3)}$$

$$\therefore k_2^2 = \frac{2m(E - V_0)}{\hbar^2} \quad \text{--- (4)}$$

Soln of eqn (3) be written as

$$\psi_{II} = C e^{ik_2 x} + D e^{-ik_2 x}$$

(represents (left to right) (transmitted)) (represents (right to left) (reflected))

Since there is no barrier in the second region.

$$\therefore \psi_{II} = C e^{ik_2 x} \quad \text{--- (B)}$$

Applying boundary condition, we get, $x=0$.

$$\psi_I \Big|_{x=0} = \psi_{II} \Big|_{x=0}$$

$$A + B = C \quad \text{--- (5)}$$

$$\frac{d\psi_I}{dx} \Big|_{x=0} = \frac{d\psi_{II}}{dx} \Big|_{x=0}$$

$$\text{or, } A e^{ik_1 x} (ik_1) + B e^{-ik_1 x} (-ik_1) = C i k_2 e^{ik_2 x}$$

$$\text{or, } i k_1 (A - B) = i k_2 C$$

$$A - B = \frac{k_2}{k_1} C \quad \text{--- (6)}$$

Adding and subtracting eqn (5) and (6) we get,

$$2A = \left(\frac{k_2 + 1}{k_1} \right) C$$

$$\Rightarrow A = \left(\frac{k_1 + k_2}{k_1} \right) \frac{C}{2} \quad \text{--- (7)}$$

$$\frac{C}{A} = \frac{2k_1}{k_1 + k_2} \quad \text{--- (8)}$$

And,

$$2B = \left(1 - \frac{k_2}{k_1} \right) C$$

$$B = \left(\frac{k_1 - k_2}{k_1} \right) \frac{C}{2}$$

$$B = \left(\frac{k_1 - k_2}{k_1} \right) \frac{A k_1}{(k_1 + k_2)} \quad \text{using (7)}$$

$$\text{or } B = \left(\frac{k_1 - k_2}{k_1 + k_2} \right) A \quad \text{--- (9)}$$

$$\Rightarrow \frac{B}{A} = \frac{k_1 - k_2}{k_1 + k_2} \quad \text{--- (10)}$$

Now, the incident prob-current density.

$$J_{inc} = \frac{-i\hbar}{2m} \left(\psi_{inc}^* \frac{\partial \psi_{inc}}{\partial x} - \psi_{inc} \frac{\partial \psi_{inc}^*}{\partial x} \right)$$

$$= \frac{-i\hbar}{2m} \left(A e^{-ik_1 x} (ik_1) e^{ik_1 x} - A e^{ik_1 x} (-ik_1) e^{-ik_1 x} \right)$$

$$= \frac{-i\hbar}{2m} \left(|A|^2 + |A|^2 \right) ik_1$$

$$J_{inc} = \frac{\hbar k_1}{m} |A|^2 \quad \text{--- (11)}$$

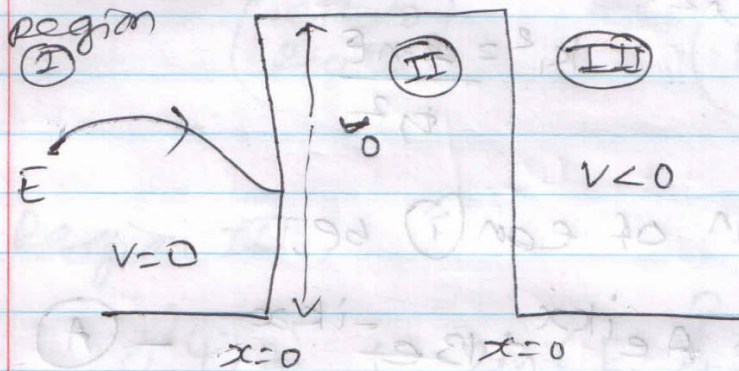
Similarly,

$$J_{ref} = -\frac{\hbar k_1}{m} |B|^2 \quad \text{--- (12)}$$

$$J_{trans} = \frac{\hbar k_2}{m} |C|^2 \quad \text{--- (13)}$$

DP Sir

Potential barrier



① $E > V_0$

Let the beam of particle incident to the barrier of width a and height V_0 . Let the energy of incident particle is greater than the height of the barrier.

Region I

$$\frac{d^2 \psi_I}{dx^2} + \frac{2m(E - V)}{\hbar^2} \psi_I = 0$$

$$\frac{d^2 \psi_I}{dx^2} + \frac{2mE}{\hbar^2} \psi_I = 0$$

$$\frac{d^2 \psi_I}{dx^2} + k_1^2 \psi_I = 0 \quad \text{--- (1)}$$

$$k_1^2 = \frac{2mE}{\hbar^2}$$

The soln of eqn (1) be,

$$\psi_I = A e^{ik_1 x} + B e^{-ik_1 x} \quad \text{--- (A)}$$

(incident) (reflected)

Region II

$$\frac{d^2 \psi_{II}}{dx^2} + 2m \frac{(E - V_0)}{\hbar^2} \psi_{II} = 0$$

$$\text{or, } \frac{d^2 \psi_{II}}{dx^2} + k_2^2 \psi_{II} = 0 \quad \text{--- (3)}$$

$$k_2^2 = \frac{2m(E - V_0)}{\hbar^2} \quad \text{--- (4)}$$

The soln of eqn (3) becomes,

$$\psi_{II} = C e^{ik_1 x} + D e^{-ik_2 x} \quad - (B)$$

(left to right)
(right to left)

Region III,

$$\frac{d^2 \psi_{III}}{dx^2} + \frac{2m(E - \overset{0}{V_1})}{\hbar^2} \psi_{III} = 0$$

$$\Rightarrow \frac{d^2 \psi_{III}}{dx^2} + k_3^2 \psi_{III} = 0 \quad - (5)$$

$$k_3^2 = \frac{2mE}{\hbar^2}$$

The soln be written as,

$$\psi_{III} = E e^{ik_3 x} + f e^{-ik_3 x}$$

$$\psi_{III} = E e^{ik_3 x}$$

Applying boundary condition,

At $x=0$,

$$\psi_I \Big|_{x=0} = \psi_{II} \Big|_{x=0}$$

$$A+B = C+D \quad \text{--- (6)}$$

$$\frac{d\psi_I}{dx} \Big|_{x=0} = \frac{d\psi_{II}}{dx} \Big|_{x=0}$$

$$\text{or, } ik_1(A-B) = ik_2(C-D)$$

$$\text{or, } A-B = \frac{k_2}{k_1}(C-D) \quad \text{--- (7)}$$

Adding & subtracting eqn (6) and (7)
we get,

$$2A = \left(1 + \frac{k_2}{k_1}\right)C + \left(1 - \frac{k_2}{k_1}\right)D$$

$$A = \left(1 + \frac{k_2}{k_1}\right) \frac{C}{2} + \left(1 - \frac{k_2}{k_1}\right) \frac{D}{2}$$

And,

$$2B = \left(1 - \frac{k_2}{k_1}\right) C + \left(1 + \frac{k_2}{k_1}\right) \frac{D}{2}$$

$$B = \left(1 - \frac{k_2}{k_1}\right) \frac{C}{2} + \left(1 + \frac{k_2}{k_1}\right) \frac{D}{2} \quad \text{--- (9)}$$

At $x=0$,

$$\psi_{II}|_{x=a} = \psi_{II}|_{x=a}$$

$$\text{or, } C e^{ik_2 a} + D e^{-ik_2 a} = E e^{ik_1 a} \quad \text{--- (10)}$$

And,

$$\left. \frac{d\psi_{II}}{dx} \right|_{x=a} = \left. \frac{d\psi_{II}}{dx} \right|_{x=a}$$

$$C i k_2 e^{ik_2 a} - D i k_2 e^{-ik_2 a} = i k_1 E e^{ik_1 a}$$

$$C e^{ik_2 a} - D e^{-ik_2 a} = \frac{k_1}{k_2} E e^{ik_1 a}$$

Adding & Sub eqn (10) & (11)

$$2C e^{ik_2 a} = \left(1 + \frac{k_1}{k_2}\right) E e^{ik_1 a}$$

$$C = \left(1 + \frac{k_1}{k_2}\right) \frac{E}{2} e^{i(k_1 - k_2)a} \quad \text{--- (12)}$$

And,

$$2D e^{-ik_2 a} = \left(1 - \frac{k_1}{k_2}\right) E e^{ik_1 a}$$

$$D = \left(1 - \frac{k_1}{k_2}\right) \frac{E}{2} e^{i(k_1 + k_2)a} \quad \text{--- (13)}$$

using the value of C and D in eqn (8) & (9), we get,

$$A = \left(1 + \frac{k_2}{k_1}\right) \left(1 + \frac{k_1}{k_2}\right) \frac{E}{4} e^{i(k_1 - k_2)a}$$

$$+ \left(1 - \frac{k_2}{k_1}\right) \left(1 - \frac{k_1}{k_2}\right) \frac{E}{4} e^{i(k_1 + k_2)a}$$

$$A = \frac{k_1}{2k_2} E \left[\left\{ 1 + \left(\frac{k_2}{k_1} \right)^2 \right\} - i \sin k_2 a + \frac{2k_2}{k_1} \cos k_2 a \right] e^{ik_1 a}$$

where,

$$\sin k_2 a = \frac{e^{ik_2 a} - e^{-ik_2 a}}{2i}$$

$$\cos k_2 a = \frac{e^{ik_2 a} + e^{-ik_2 a}}{2}$$

$$\frac{E}{A} = \frac{2k_2/k_1}{\left[-i \left(1 + \left(\frac{k_2}{k_1} \right)^2 \right) \sin k_2 a + \frac{2k_2}{k_1} \cos k_2 a \right] e^{ik_1 a}}$$

Now,

Transmission coefficient.

$$T = \left| \frac{E}{A} \right|^2 = \frac{E}{A} \left(\frac{E}{A} \right)^*$$

$$T = \frac{4k_1^2 k_2^2}{(k_1 - k_2)^2 \sin^2 k_2 a + 4k_1^2 k_2^2} \quad (14)$$

And

$$\frac{B}{E} = \frac{-i \left[1 - \left(\frac{k_2}{k_1} \right)^2 e^{ik_1 a} \sin k_2 a \right]}{2 \frac{k_2}{k_1}} \quad (15)$$

Now,

$$\frac{B}{E} \times \frac{E}{A} = \frac{-i \left\{ 1 - \left(\frac{k_2}{k_1} \right)^2 \right\} e^{ik_1 a} \sin k_2 a}{\left\{ \left(1 + \left(\frac{k_2}{k_1} \right)^2 \right) \left[(-i \sin k_2 a) + 2 \frac{k_2 \cos k_2 a}{k_1} \right] \right\}}$$

So,

Reflection coefficient

$$R = \left(\frac{B}{A} \right)^2 = \frac{B}{A} \left(\frac{B}{A} \right)^*$$

$$R = \frac{(k_1 - k_2)^2 \sin^2 k_2 a}{(k_1 - k_2)^2 \sin^2 k_2 a + 4k_1^2 k_2^2}$$

Trans

$$R+T=1$$

Special case,

$$T = \frac{4k_1^2 k_2^2}{(k_1^2 - k_2^2)^2 \sin^2 k_2 a + 4k_1^2 k_2^2}$$

special case,

$$T = \frac{4k_1^2 k_2^2}{(k_1^2 - k_2^2) \sin^2 k_2 a + 4k_1^2 k_2^2}$$

for $\sin^2 k_2 a = 0$

$$\Rightarrow \sin k_2 a = 0$$

$$k_2 a = n\pi$$

$$a = \frac{n\pi}{k_2} ; n=0, 1, 2, 3, \dots$$

$$a = 0 ; \frac{\pi}{k_2}, \frac{2\pi}{k_2}, \frac{3\pi}{k_2} \dots$$

(ii) $E < V_0$

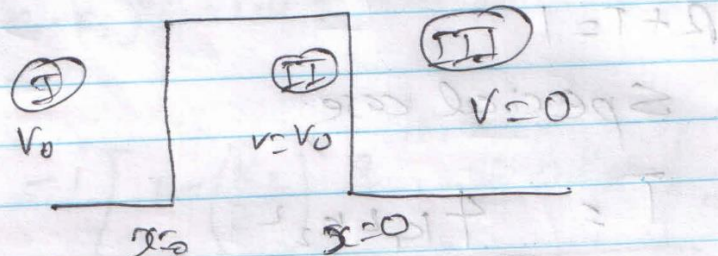


fig: Tunneling of barrier.

Even for $E < V_0$, a few beam of particle can penetrate then barrier is called ϕ tunneling effects.

$$R = \frac{V_0^2 \sinh^2 \beta a}{4E(V_0 - E) \left(1 + \frac{V_0^2 \sinh^2 \beta a}{4E(V_0 - E)} \right)}$$

$$\beta^2 = \frac{2m}{\hbar^2} (V_0 - E)$$

$$T = \frac{1}{1 + \frac{V_0^2 \sinh^2 \beta a}{4E(V_0 - E)}}$$

$$R + T = 1$$

left of DP

The reflection and transmission coefficient (T) be written as,

$$R = \frac{J_{ref}}{J_{inc}} \quad T = \frac{J_{trans}}{J_{inc}}$$

$$R = \frac{\frac{\hbar k_1}{m} |B|^2}{\frac{\hbar k_1}{m} |A|^2}$$

$$\text{or, } R = \left| \frac{B}{A} \right|^2 = \frac{B}{A} \left(\frac{B}{A} \right)^*$$

$$= \left(\frac{k_1 - k_2}{k_1 + k_2} \right) \left(\frac{k_1 - k_2}{k_1 + k_2} \right)^* = \left(\frac{k_1 - k_2}{k_1 + k_2} \right)^2$$

— (14)

$$\text{Q } T = \frac{J_{trans}}{J_{inc}} = \frac{\frac{\hbar k_2}{m} |C|^2}{\frac{\hbar k_1}{m} |A|^2}$$

$$\text{Q } T = \frac{k_2}{k_1} \left| \frac{C}{A} \right|^2$$

$$\therefore T = \frac{k_2}{k_1} \left(\frac{2k_1}{k_1 + k_2} \right)^2 = 4 \frac{k_1 k_2}{(k_1 + k_2)^2}$$

Now,

$$R+T = \frac{\left(\frac{k_1 k_2}{k_1 + k_2} \right)^2 + 4 k_1 k_2}{(k_1 + k_2)^2}$$

$$R+T = \frac{(k_1 - k_2)^2 + 4 k_1 k_2}{(k_1 + k_2)^2}$$

$$R+T = \frac{(k_1 + k_2)^2}{(k_1 + k_2)^2}$$

$$\therefore R+T = 1$$

$$E < V_0$$

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After solving the solⁿ of the eqn, we get

$$\Theta(\theta) = \left\{ \frac{(2l+1)(l-m)!}{2(l+m)!} \right\}^{\frac{1}{2}} P_l^m(\cos\theta)$$

where

$P_l^m(\cos\theta)$ is Legendre Polynomial.

Then,

$$\begin{aligned} \Psi &= \Theta(\theta) \Phi(\phi) \\ &= \left[\frac{(2l+1)(l-m)!}{2(l+m)!} \right]^{\frac{1}{2}} P_l^m(\cos\theta) \frac{1}{\sqrt{2\pi}} e^{im\phi} \end{aligned}$$

with

$$E = \frac{\hbar^2}{2I} l(l+1)$$

when $l = 0, 1, 2, 3, \dots$ is called rotational quantum number

where $l=0, E_0=0$

$$l=1 \quad E_1 = \frac{\hbar^2}{2I} \cdot 2 = 2B \text{ (say)}$$

$$l=2 \quad E_2 = \frac{\hbar^2}{2I} \cdot 6 = 6B$$

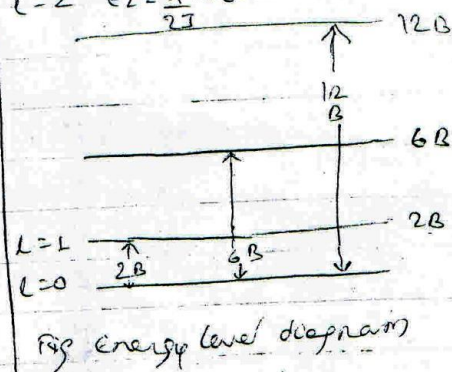
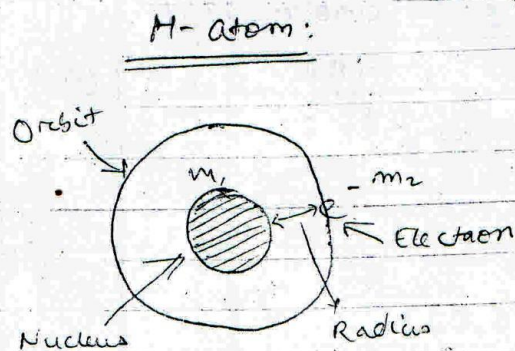


Fig: H-atom (similar to two body problem)

For H-atom, Schrodinger wave equation be written as

$$\nabla^2 \psi + \frac{2m}{\hbar^2} (E - V) \psi = 0$$

$$0, \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} +$$

$$\frac{2\mu}{\hbar^2} (E - V) \psi = 0$$

$$\mu = \frac{m_1 m_2}{m_1 + m_2}$$

Let $\psi(r, \theta, \phi) = R(r) \overset{\substack{\uparrow \\ \text{Radial Part}}}{Y(\theta, \phi)}$ $\overset{\substack{\uparrow \\ \text{Angular part}}}$

$$\frac{Y(\theta, \phi)}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \psi}{\partial r} \right) + \frac{R(r)}{r^2 \sin^2 \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial Y(\theta, \phi)}{\partial \theta} \right) + \frac{R(r)}{r^2 \sin^2 \theta} \frac{\partial^2 Y(\theta, \phi)}{\partial \phi^2} + \frac{2\mu}{\hbar^2} (E - V) R(r) Y(\theta, \phi) = 0$$

Multiplying by r^2 and Dividing by $R(r) Y(\theta, \phi)$, we get

$$\frac{1}{R(r)} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R(r)}{\partial r} \right) + \frac{1}{\sin^2 \theta Y(\theta, \phi)} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial Y(\theta, \phi)}{\partial \theta} \right) + \frac{1}{Y(\theta, \phi) \sin^2 \theta} \frac{\partial^2 Y(\theta, \phi)}{\partial \phi^2} + \frac{2\mu r^2 (E - V)}{\hbar^2} = 0$$

$$\frac{1}{R(r)} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R(r)}{\partial r} \right) + \frac{2\mu r^2 (E - V)}{\hbar^2} = - \frac{1}{Y(\theta, \phi)} \left[\frac{1}{\sin^2 \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial Y(\theta, \phi)}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y(\theta, \phi)}{\partial \phi^2} \right]$$

$$\frac{1}{R(r)} \left[\frac{\partial}{\partial r} \left(r^2 \frac{\partial R(r)}{\partial r} \right) + \frac{2\mu r^2 (E - V) R(r)}{\hbar^2} \right] = - \frac{1}{Y(\theta, \phi)} \left[\frac{1}{\sin^2 \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial Y(\theta, \phi)}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y(\theta, \phi)}{\partial \phi^2} \right] = \lambda \text{ (say)}$$

So,

$$\frac{\partial}{\partial r} \left(r^2 \frac{\partial R(r)}{\partial r} \right) + \frac{2\mu r^2 (E - V) R(r) - \lambda R(r)}{\hbar^2} = 0 \quad \text{--- (1)}$$

And,

$$\left[\frac{1}{\sin \theta} \cdot \frac{\partial}{\partial \theta} \left(\sin \theta \cdot \frac{\partial Y(\theta, \phi)}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y(\theta, \phi)}{\partial \phi^2} + \lambda(\theta, \phi) \right] = 0 \quad \text{--- (2)}$$

Put $Y(\theta, \phi) = H(\theta) \Phi(\phi)$

after solving

The solution of eqn (1) and (2) be written as

$$R(r) = \left[\frac{2^{L+1} (m-L-1)!}{2n\Gamma(m+L)!} \right]^{\frac{1}{2}} \frac{1}{2} e^{-\frac{r}{2}} r^L L_{m+L}^{2L+1}(r) \\ - \left[\frac{(2L+1)(L-m)!}{2(L+m)!} \right]^{\frac{1}{2}} P_L^m(\cos \theta) \frac{1}{\sqrt{2\pi}} e^{im\phi}$$

$\nabla^2 = \nabla \cdot \nabla$

$KE + PE$

$\frac{p^2}{2m} + V$

$-\frac{\hbar^2}{2m} \nabla^2 + V$

$H = -\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) - \frac{e^2}{4\pi\epsilon_0 r}$

Hamiltonian or ^{total} energy operator and its value

$\hat{H} = \hat{K} + \hat{P}$

HARMONIC OSCILLATOR

The system in which acceleration varies -ve of the displacement is called harmonic oscillator.

- e.g.,
- simple pendulum
 - Compound Pendulum
 - loaded spring etc.

For this system,

$$PE = \frac{1}{2} kx^2$$

$$= \frac{1}{2} m\omega^2 x^2$$

$$KE = \frac{1}{2} mv^2$$

Again,

$$F \propto -x$$

or, $F = -kx$; k is called spring constant

$$\text{or, } ma = -kx$$

$$a = -\left(\frac{k}{m}\right)x$$

$$= -\omega^2 x$$

$$\Rightarrow \omega^2 = \frac{k}{m}$$

$$\omega = \sqrt{\frac{k}{m}}$$

$$2\pi f = \sqrt{\frac{k}{m}}$$

$$f = \frac{1}{2\pi} \sqrt{\frac{k}{m}} \quad \Bigg| \Rightarrow T = 2\pi \sqrt{\frac{m}{k}}$$

For simple type of harmonic oscillation,

$$y = A \sin \omega t$$

$$a. \frac{dy}{dt} = A \omega \cos \omega t$$

$$v = A \omega \cos \omega t$$

$$\Rightarrow \frac{dv}{dt} = -A \omega^2 \sin \omega t$$

$$\therefore \text{acceleration} = -\omega^2 A \sin \omega t$$

$$a. \boxed{a = -\omega^2 y}$$

$$v = A \omega \sqrt{1 - \sin^2 \omega t}$$

$$= A \omega \sqrt{1 - \frac{y^2}{A^2}}$$

$$= \omega \sqrt{A^2 - y^2}$$

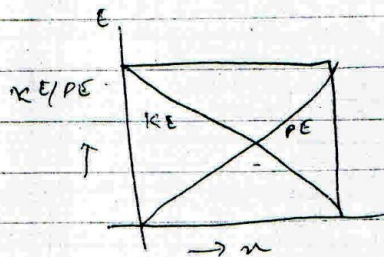
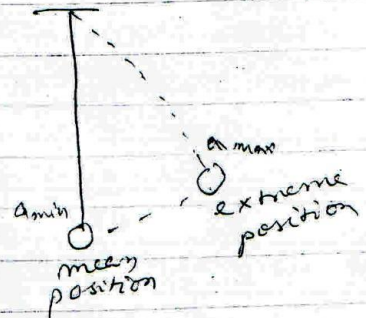
Again,

The total energy of H.O,

$$E = \frac{1}{2} m v^2 + \frac{1}{2} m \omega^2 x^2$$

$$= \frac{1}{2} m \omega^2 (A^2 - x^2) + \frac{1}{2} m \omega^2 x^2$$

$$E = \frac{1}{2} m \omega^2 A^2$$



QUANTUM MECHANICAL TREATMENT

The Schrodinger wave equation of Harmonic oscillator is written as

$$\frac{d^2 \psi}{dx^2} + \frac{2m}{\hbar^2} (E - V) \psi = 0$$

$$\text{or, } \frac{d^2 \psi}{dx^2} + \frac{2m}{\hbar^2} \left(E - \frac{1}{2} m \omega^2 x^2 \right) \psi = 0$$

$$\text{or, } \frac{d^2 \psi}{dx^2} + \left(\frac{2mE}{\hbar^2} - \frac{m^2 \omega^2 x^2}{\hbar^2} \right) \psi = 0$$

$$\text{Let } y = \sqrt{\frac{m\omega}{\hbar}} \cdot x$$

$$\text{or, } y = \sqrt{\alpha} x, \quad \alpha = \frac{m\omega}{\hbar}$$

$$\Rightarrow \frac{dy}{dx} = \sqrt{\alpha}$$

$$= \sqrt{\frac{m\omega}{\hbar}}$$

$$\Rightarrow \frac{dx}{dy} = \sqrt{\frac{\hbar}{m\omega}}$$

Now,

$$\frac{d\psi}{dx} = \frac{d\psi}{dy} \left(\frac{dy}{dx} \right)$$

$$= \frac{d\psi}{dy} \sqrt{\frac{m\omega}{\hbar}}$$

$$\text{or, } \frac{d^2 \psi}{dx^2} = \frac{d^2 \psi}{dy^2} \left(\frac{dy}{dx} \right)^2 \sqrt{\frac{m\omega}{\hbar}}$$

$$= \frac{d^2 \psi}{dy^2} \left(\frac{dy}{dx} \right)^2 \sqrt{\frac{m\omega}{\hbar}}$$

$$n, \frac{d^2 \psi}{dx^2} = \frac{d^2 \psi}{dy^2} \left(\frac{m \omega}{\hbar} \right)$$

changing the x variable into y , we get

$$\frac{\hbar \omega}{\hbar} \frac{d^2 \psi}{dy^2} + \left(\frac{2mE}{\hbar^2} - \frac{m^2 \omega^2}{\hbar^2} \frac{\hbar}{m \omega} y^2 \right) \psi = 0$$

$$n, \frac{d^2 \psi}{dy^2} + \left(\frac{2E}{\hbar \omega} - y^2 \right) \psi = 0$$

$$n, \frac{d^2 \psi}{dy^2} + (\lambda - y^2) \psi = 0$$

$$\text{where } \lambda = \frac{2E}{\hbar \omega}$$

$$E = \frac{\hbar \omega \lambda}{2}$$

Solving this differential equation with asymptotic soln we get, its solution in terms of Hermite polynomials.

$$\psi(y) = H(y) e^{-\frac{y^2}{2}}$$

↓

$$\psi(y) = \left\{ a_0 \left[1 + \frac{(1-\lambda)y^2}{2!} + \frac{(1-\lambda)(5-\lambda)y^4}{4!} + \frac{(1-\lambda)(5-\lambda)(9-\lambda)y^6}{6!} + \dots \right] + a_1 \left[y + \frac{(3-\lambda)y^3}{3!} + \frac{(3-\lambda)(7-\lambda)y^5}{5!} + \dots \right] \right\} e^{-\frac{y^2}{2}}$$

And,

$$\lambda = 2n+1$$

Then,

$$\lambda = \frac{2E}{\hbar\omega}$$

$$n, (2n+1) = \frac{2E}{\hbar\omega}$$

$$n, E = \frac{(2n+1)\hbar\omega}{2}$$
$$= \left(n + \frac{1}{2}\right)\hbar\omega$$

$$E = \left(n + \frac{1}{2}\right)\hbar\omega, n = 0, 1, 2, 3, \dots$$

In general,

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega$$

for $n=0$,

$$E_0 = \frac{1}{2}\hbar\omega$$

$$= \frac{1}{2} \times \frac{h}{2\pi} \cdot 2\pi f$$

$$E_0 = \frac{1}{2}hf$$

zero point energy

$$n=1$$

$$E_1 = \frac{3}{2}\hbar\omega$$

1st energy state

for $n=2$,

$$E_2 = \frac{5}{2} h \omega$$

2nd Excited energy.

A Pendulum with a length of 1m has a bob of mass 0.1 kg.
What is the zero point energy? $[1.65 \times 10^{-34} \text{ J}]$

$$t = 2\pi \sqrt{\frac{l}{g}}$$

$$f = \frac{1}{t}$$

$$E_0 = \frac{1}{2} h \omega$$

$$= \frac{1}{2} h f = \frac{1}{2} \times 6.62 \times 10^{-34} \times 0.1 =$$

Q. A particle of mass 10^{-6} kg is attached to a spring of spring constant 10^{-3} Nm^{-1} . Calculate its zero point energy and classical value of amplitude of zero point vibration.

So,

$$f = \frac{1}{2\pi} \sqrt{\frac{k}{m}}$$

$$= \frac{1}{2\pi} \sqrt{\frac{10^{-3}}{10^{-6}}}$$

$$= 5.033$$

$$E_0 = \frac{1}{2} h \times 5.033$$

$$= 1.666 \times 10^{-33} \text{ J}$$

for classical amplitude

$$E_3 = \frac{1}{2} m \omega^2 A^2$$

$$\therefore A = \sqrt{\frac{2E_0}{m\omega^2}}$$

- Q. Calculate the zero point energy of a system consisting a mass of 1 gm connected to a fixed point by spring which is stretched 1 cm, by a force of 10^4 dynes. The particle is constrained to move along x-direction.

Soln

$$F = kx$$

$$k = \frac{10^4}{1}$$

$$= 10^4 \text{ dyne cm}^{-1}$$

$$f = \frac{1}{2\pi} \sqrt{\frac{k}{m}}$$

$$= \frac{1}{2\pi} \sqrt{\frac{10^4}{1}}$$

$$= 15.92$$

$$E_0 = \frac{1}{2} h \times 15.92$$

$$= 8.27 \times 10^{-33} \text{ erg}$$

An electron is put in a cubical box of each side $1 \text{ \AA}$. Calculate its momentum and energy per first excited states.

A particle of K.E 9 eV incident on a potential step of height 5 eV . Find the value of reflection coefficient.

①.

$$a = 1 \text{ \AA} = 10^{-10} \text{ m}$$

$$E_{n_x, n_y, n_z} = \frac{h^2 \pi^2}{2m a^2} [n_x^2 + n_y^2 + n_z^2]$$

for G.S

$$E_{111} = \frac{h^2 \pi^2}{2m a^2} (3)$$

for 1st E.S

$$E_{112} = E_{211} = E_{121} = \frac{h^2 \pi^2}{2m a^2} [1^2 + 2^2 + 1^2]$$

for momentum,

$$k_x = \frac{n\pi}{a}, \quad k_y = \frac{n\pi}{a}, \quad k_z = \frac{n\pi}{a}$$

Then,

$$p = \hbar k$$

$$p = \hbar (k_x + k_y + k_z)$$

for General.

$$p_x p_y p_z = \hbar \left(\frac{n_x \pi}{a} + \frac{n_y \pi}{a} + \frac{n_z \pi}{a} \right)$$

✓

For G.S.,

$$p_{111} = \frac{\hbar \pi}{a} [3]$$

For 1st E.S.,

$$p_{121} = p_{211} = p_{21} = \frac{\hbar \pi}{a} [4]$$

Q.7

Where will the particle be most likely found if the normal wave function of a particle moving on a straight line is

$$\psi(x) = \left(\frac{\sqrt{\pi}}{2} \right) e^{-(ax^2 - i \frac{p_x}{\hbar})}$$

Soln

The probability of finding the particle in a region is given by

$$P = \psi^* \psi = |\psi|^2$$

$$= \left(\frac{\sqrt{\pi}}{2} \right)^2 e^{-(ax^2 - i \frac{p_x}{\hbar})} \cdot e^{-(ax^2 + i \frac{p_x}{\hbar})}$$

$$= \frac{\pi}{4} \cdot e^{-2ax^2}$$

For maximum probability,

$$\frac{dP}{dx} = 0$$

$$\text{or } \frac{d}{dx} \left(\frac{\pi}{4} \cdot e^{-2ax^2} \right) = 0$$